



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 07:06 pm GMT

PDB ID : 3HWS
Title : Crystal structure of nucleotide-bound hexameric ClpX
Authors : Glynn, S.E.; Martin, A.; Baker, T.A.; Sauer, R.T.
Deposited on : 2009-06-18
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

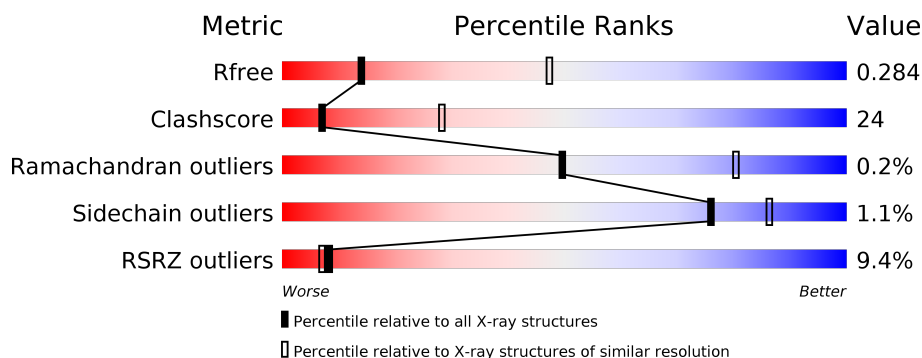
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1008 (3.30-3.22)
Clashscore	122126	1066 (3.30-3.22)
Ramachandran outliers	120053	1046 (3.30-3.22)
Sidechain outliers	120020	1045 (3.30-3.22)
RSRZ outliers	108989	1993 (3.32-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div>8%</div> <div> <div>54%</div> <div>33%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	363	<div> <div>7%</div> <div> <div>54%</div> <div>32%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	363	<div> <div>6%</div> <div> <div>53%</div> <div>30%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	363	<div> <div>10%</div> <div> <div>52%</div> <div>35%</div> <div>13%</div> </div> </div>
1	E	363	<div> <div>9%</div> <div> <div>50%</div> <div>35%</div> <div>•</div> <div>14%</div> </div> </div>
1	F	363	<div> <div>9%</div> <div> <div>50%</div> <div>36%</div> <div>•</div> <div>13%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	E	603	-	-	X	-
3	SO4	B	708	-	-	-	X
3	SO4	D	710	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP-dependent Clp protease ATP-binding subunit clpX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2381	1514	396	465	6			
1	B	315	Total	C	N	O	S	0	0	0
			2388	1519	405	458	6			
1	C	307	Total	C	N	O	S	0	0	0
			2333	1485	392	450	6			
1	D	316	Total	C	N	O	S	0	0	0
			2333	1485	393	449	6			
1	E	313	Total	C	N	O	S	0	0	0
			2310	1468	384	452	6			
1	F	314	Total	C	N	O	S	0	0	0
			2367	1502	398	461	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLN	GLU	ENGINEERED	UNP P0A6H1
A	408	GLU	LYS	ENGINEERED	UNP P0A6H1
B	185	GLN	GLU	ENGINEERED	UNP P0A6H1
B	408	GLU	LYS	ENGINEERED	UNP P0A6H1
C	185	GLN	GLU	ENGINEERED	UNP P0A6H1
C	408	GLU	LYS	ENGINEERED	UNP P0A6H1
D	185	GLN	GLU	ENGINEERED	UNP P0A6H1
D	408	GLU	LYS	ENGINEERED	UNP P0A6H1
E	185	GLN	GLU	ENGINEERED	UNP P0A6H1
E	408	GLU	LYS	ENGINEERED	UNP P0A6H1
F	185	GLN	GLU	ENGINEERED	UNP P0A6H1
F	408	GLU	LYS	ENGINEERED	UNP P0A6H1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

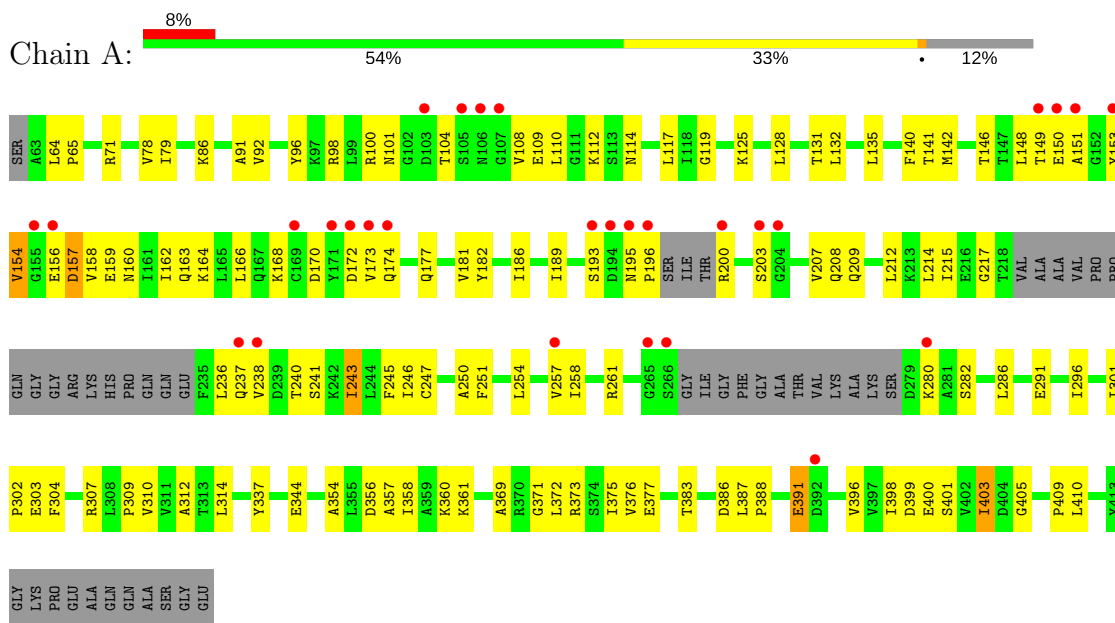
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 1 1	0	0
5	C	3	Total O 3 3	0	0
5	E	1	Total O 1 1	0	0

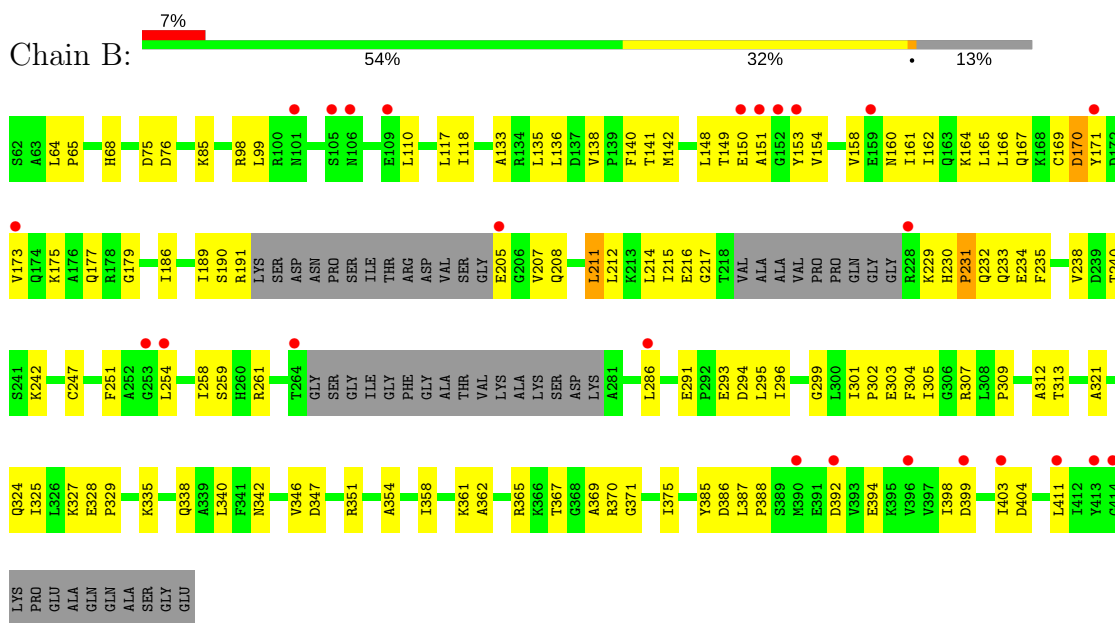
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

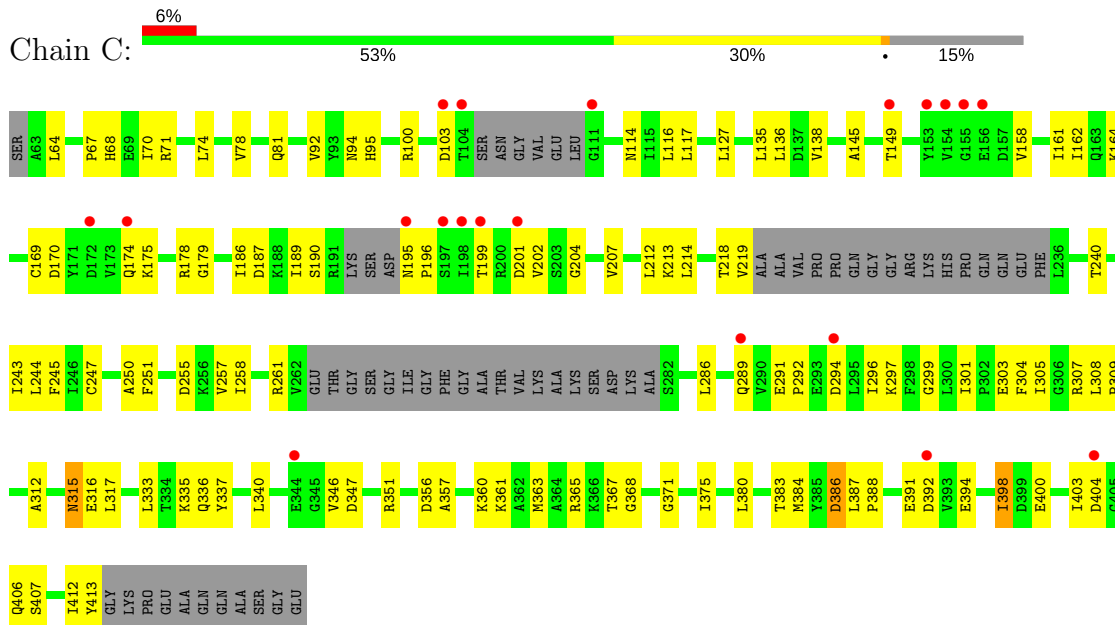
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX



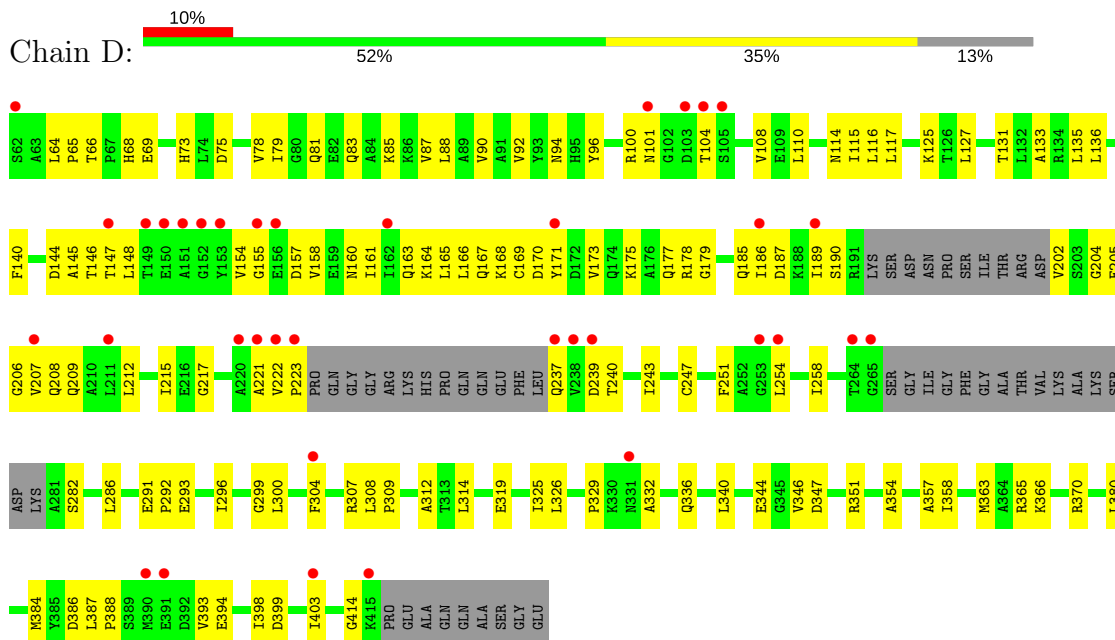
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX



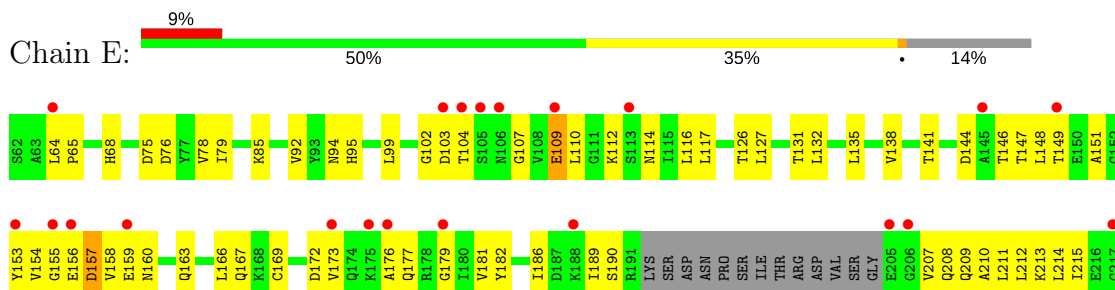
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX

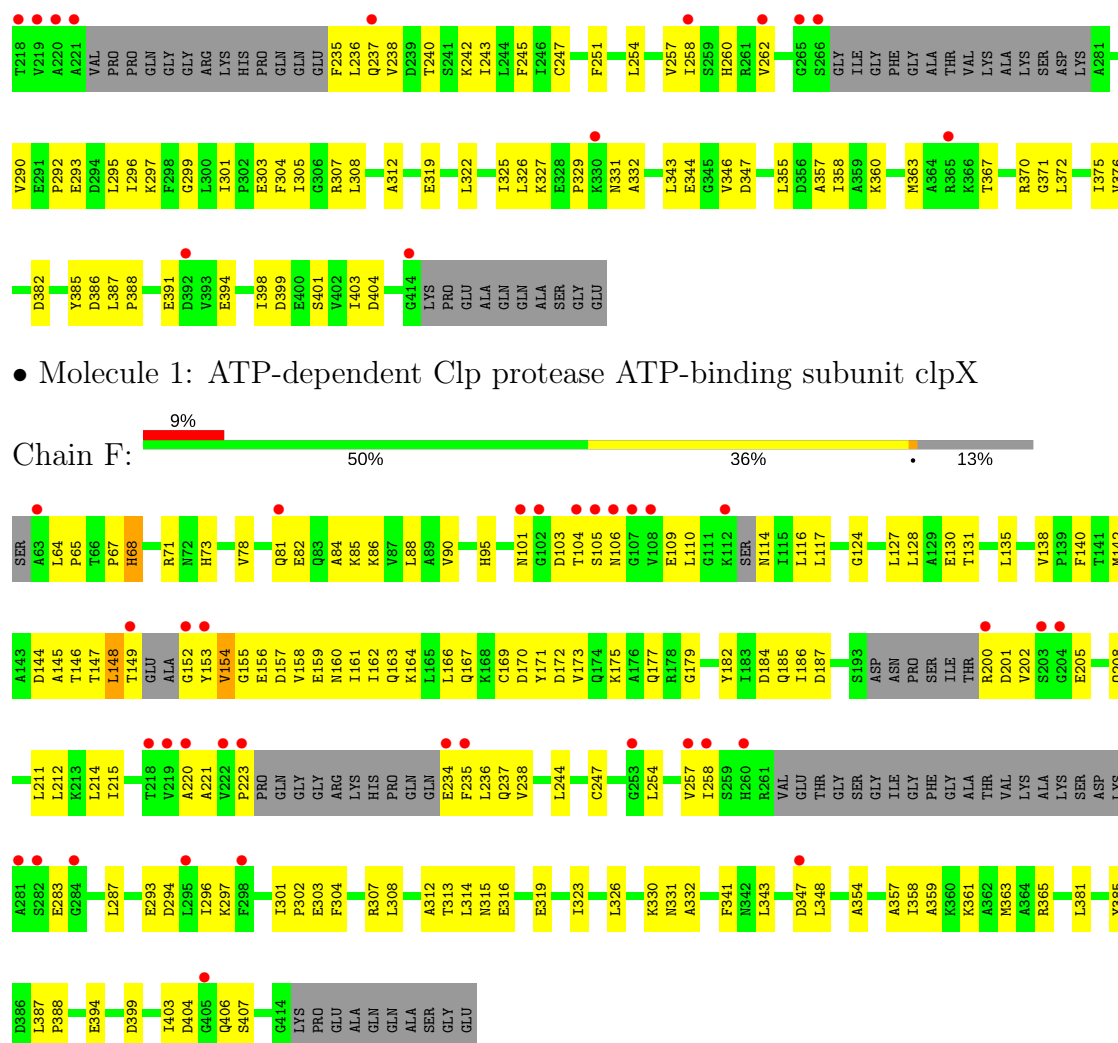


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX



• Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX





- Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.09Å 178.50Å 201.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.08 – 3.25 45.08 – 3.22	Depositor EDS
% Data completeness (in resolution range)	96.2 (45.08-3.25) 98.7 (45.08-3.22)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.282 0.239 , 0.284	Depositor DCC
R_{free} test set	1573 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 95.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14292	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/2408	0.41	0/3265
1	B	0.22	0/2416	0.39	0/3268
1	C	0.22	0/2359	0.39	0/3193
1	D	0.22	0/2360	0.39	0/3201
1	E	0.25	0/2337	0.44	0/3172
1	F	0.24	0/2393	0.40	0/3239
All	All	0.23	0/14273	0.41	0/19338

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2381	0	2363	115	0
1	B	2388	0	2417	104	0
1	C	2333	0	2370	105	0
1	D	2333	0	2317	118	0
1	E	2310	0	2279	170	0
1	F	2367	0	2362	125	0
2	A	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	3	0
2	D	27	0	12	4	0
2	E	27	0	12	9	0
3	A	15	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	1	0
5	E	1	0	0	0	0
All	All	14292	0	14156	693	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:THR:HG21	1:F:301:ILE:HG22	1.35	1.09
1:D:148:LEU:HD21	1:D:158:VAL:HG12	1.34	1.08
1:E:303:GLU:HG2	1:E:307:ARG:HH22	1.13	1.08
1:B:161:ILE:HA	1:B:164:LYS:HE2	1.35	1.07
1:A:150:GLU:HA	1:A:203:SER:CB	1.87	1.05
1:A:150:GLU:CA	1:A:203:SER:HB2	1.88	1.02
1:A:154:VAL:HA	1:A:157:ASP:HB3	1.41	1.01
1:A:151:ALA:HB3	1:A:154:VAL:HB	1.45	0.98
1:E:148:LEU:HA	1:E:154:VAL:HG21	1.41	0.98
1:E:177:GLN:HB3	1:E:238:VAL:HG21	1.45	0.98
1:F:152:GLY:O	1:F:154:VAL:HG23	1.64	0.97
1:A:150:GLU:HA	1:A:203:SER:HB2	0.99	0.96
1:B:186:ILE:HG13	1:B:247:CYS:HB3	1.49	0.92
1:D:186:ILE:HG13	1:D:247:CYS:HB3	1.52	0.92
1:B:229:LYS:HD2	1:B:233:GLN:HB3	1.52	0.91
1:F:158:VAL:HB	1:F:214:LEU:HD23	1.53	0.91
1:B:148:LEU:HB3	1:B:154:VAL:HG23	1.54	0.90
1:E:212:LEU:HD22	1:E:307:ARG:HH21	1.37	0.89
1:E:173:VAL:HG13	1:E:238:VAL:HB	1.54	0.89
1:E:151:ALA:O	1:E:154:VAL:HG12	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASP:O	1:D:147:THR:HG22	1.74	0.87
1:A:186:ILE:HG13	1:A:247:CYS:HB3	1.58	0.85
1:C:169:CYS:SG	1:C:175:LYS:HB2	2.17	0.85
1:A:148:LEU:O	1:A:154:VAL:HG11	1.77	0.85
1:E:154:VAL:O	1:E:158:VAL:HG23	1.76	0.83
1:A:357:ALA:HB1	1:A:403:ILE:HG23	1.58	0.83
1:D:155:GLY:O	1:D:158:VAL:HG22	1.78	0.83
1:E:148:LEU:CA	1:E:154:VAL:HG21	2.08	0.83
1:A:148:LEU:HA	1:A:154:VAL:HG21	1.61	0.83
1:A:280:LYS:CB	1:A:286:LEU:HD11	2.09	0.82
1:F:81:GLN:HE22	1:F:316:GLU:H	1.26	0.81
1:A:215:ILE:HG21	1:A:307:ARG:HB3	1.61	0.81
1:E:357:ALA:HB1	1:E:403:ILE:HG23	1.62	0.80
1:F:173:VAL:HG13	1:F:238:VAL:HG22	1.62	0.80
1:C:186:ILE:HG13	1:C:247:CYS:HB3	1.61	0.79
1:F:71:ARG:HG3	1:F:85:LYS:HB3	1.65	0.78
1:A:337:TYR:OH	1:A:377:GLU:HG2	1.82	0.78
1:E:144:ASP:O	1:E:148:LEU:HG	1.84	0.78
1:E:147:THR:CG2	1:F:301:ILE:HG22	2.14	0.77
1:A:114:ASN:ND2	1:A:215:ILE:HG23	2.01	0.76
1:E:157:ASP:O	1:E:160:ASN:HB3	1.85	0.76
1:C:315:ASN:H	1:C:315:ASN:HD22	1.31	0.75
1:E:127:LEU:HD22	2:E:603:ADP:H2'	1.67	0.75
1:E:157:ASP:OD1	1:E:157:ASP:C	2.23	0.75
1:A:157:ASP:O	1:A:160:ASN:HB3	1.86	0.75
1:A:149:THR:HA	1:A:207:VAL:HG21	1.68	0.75
1:E:303:GLU:HG2	1:E:307:ARG:NH2	1.98	0.75
1:B:169:CYS:SG	1:B:175:LYS:HB2	2.26	0.75
1:A:214:LEU:HD22	1:A:240:THR:HG21	1.68	0.74
1:E:156:GLU:O	1:E:159:GLU:HG2	1.87	0.74
1:B:64:LEU:HD12	1:B:65:PRO:HD2	1.67	0.74
1:D:64:LEU:HD12	1:D:65:PRO:HD2	1.69	0.73
1:E:64:LEU:HD12	1:E:65:PRO:HD2	1.69	0.73
1:D:217:GLY:HA2	1:D:240:THR:OG1	1.88	0.73
1:A:399:ASP:O	1:A:403:ILE:HG12	1.89	0.73
1:B:229:LYS:HD2	1:B:233:GLN:CB	2.19	0.72
1:F:144:ASP:OD1	1:F:185:GLN:HG3	1.89	0.72
1:D:357:ALA:HB1	1:D:403:ILE:HG12	1.72	0.72
1:A:373:ARG:HD3	1:B:309:PRO:HB3	1.72	0.72
1:C:175:LYS:HD3	1:C:178:ARG:HH12	1.51	0.72
1:D:189:ILE:HD11	1:D:204:GLY:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:LYS:O	1:D:167:GLN:HG2	1.89	0.71
1:E:236:LEU:HD23	1:E:236:LEU:H	1.55	0.71
1:B:164:LYS:HG2	1:C:213:LYS:HD2	1.73	0.71
1:E:148:LEU:O	1:E:154:VAL:HG11	1.91	0.71
1:F:81:GLN:NE2	1:F:316:GLU:H	1.88	0.70
1:F:211:LEU:O	1:F:214:LEU:HG	1.90	0.70
1:F:158:VAL:HB	1:F:214:LEU:CD2	2.21	0.70
1:B:233:GLN:CD	1:B:234:GLU:H	1.94	0.70
1:D:64:LEU:HB2	1:D:100:ARG:HH11	1.55	0.70
1:A:173:VAL:HG13	1:A:238:VAL:HG22	1.74	0.70
1:F:114:ASN:HB3	1:F:308:LEU:HD13	1.74	0.70
1:B:230:HIS:N	1:B:231:PRO:HD2	2.07	0.69
1:E:399:ASP:O	1:E:403:ILE:HG12	1.92	0.69
1:D:144:ASP:HB3	1:D:147:THR:HG22	1.73	0.69
1:F:162:ILE:O	1:F:166:LEU:HD12	1.92	0.69
1:B:212:LEU:CD1	1:B:304:PHE:HA	2.22	0.69
1:B:158:VAL:HG13	1:B:214:LEU:HD22	1.74	0.69
1:C:186:ILE:O	1:C:189:ILE:HG12	1.93	0.69
1:D:169:CYS:SG	1:D:175:LYS:HB2	2.32	0.69
1:B:205:GLU:HA	1:B:208:GLN:HG3	1.74	0.69
1:A:112:LYS:HE3	1:A:307:ARG:HE	1.56	0.68
1:B:160:ASN:O	1:B:164:LYS:HG3	1.93	0.68
1:B:150:GLU:O	1:C:196:PRO:HG3	1.92	0.68
1:A:151:ALA:HB2	1:A:153:TYR:CZ	2.29	0.68
1:A:212:LEU:CD1	1:A:307:ARG:HG3	2.22	0.68
1:B:211:LEU:O	1:B:215:ILE:HG12	1.93	0.68
1:A:149:THR:HA	1:A:207:VAL:CG2	2.24	0.68
1:D:66:THR:HG23	1:D:69:GLU:H	1.58	0.68
1:F:236:LEU:H	1:F:236:LEU:HD23	1.58	0.68
1:B:365:ARG:HG3	1:B:367:THR:HG23	1.76	0.68
1:B:212:LEU:HD11	1:B:303:GLU:O	1.93	0.67
1:C:158:VAL:HG11	1:C:214:LEU:HB2	1.75	0.67
1:C:400:GLU:HB2	1:C:406:GLN:HE21	1.59	0.67
1:B:138:VAL:HG13	1:B:179:GLY:HA2	1.77	0.67
1:A:217:GLY:HA2	1:A:240:THR:OG1	1.95	0.67
1:D:131:THR:O	1:D:135:LEU:HG	1.94	0.67
1:B:149:THR:HA	1:B:207:VAL:HG21	1.76	0.67
1:D:116:LEU:HB2	1:D:308:LEU:HD23	1.75	0.67
1:A:243:ILE:HD11	1:A:245:PHE:CZ	2.29	0.67
1:A:212:LEU:HD11	1:A:307:ARG:HG3	1.77	0.67
1:E:388:PRO:HG2	1:F:67:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ILE:HD11	1:C:214:LEU:HD22	1.76	0.66
1:A:282:SER:O	1:A:286:LEU:HD13	1.95	0.66
1:B:327:LYS:O	1:B:335:LYS:HE3	1.95	0.66
1:D:291:GLU:HG3	1:D:292:PRO:HD2	1.77	0.66
1:F:81:GLN:HE22	1:F:315:ASN:N	1.94	0.66
1:B:177:GLN:HG3	1:B:238:VAL:HG23	1.78	0.65
1:B:141:THR:HG22	1:B:165:LEU:HD13	1.78	0.65
1:F:357:ALA:HB1	1:F:403:ILE:HG23	1.79	0.65
1:F:399:ASP:O	1:F:403:ILE:HG12	1.96	0.65
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.79	0.65
1:D:64:LEU:HB2	1:D:100:ARG:NH1	2.11	0.65
1:C:81:GLN:HE22	1:C:316:GLU:H	1.44	0.65
1:E:104:THR:HG21	1:E:109:GLU:N	2.11	0.65
1:C:158:VAL:O	1:C:161:ILE:HG12	1.97	0.65
1:E:104:THR:CG2	1:E:109:GLU:HB2	2.27	0.65
1:E:367:THR:HG21	1:E:371:GLY:HA3	1.79	0.65
1:E:370:ARG:HG2	2:E:603:ADP:H5'2	1.79	0.65
1:E:169:CYS:SG	1:E:176:ALA:HB2	2.37	0.65
1:A:117:LEU:HD23	1:A:312:ALA:HB3	1.78	0.64
1:E:149:THR:HA	1:E:207:VAL:HG11	1.78	0.64
1:B:291:GLU:HB2	1:B:293:GLU:HG2	1.79	0.64
1:E:301:ILE:HG13	1:E:304:PHE:H	1.61	0.64
1:E:147:THR:HG21	1:F:301:ILE:CG2	2.21	0.64
1:A:146:THR:O	1:A:149:THR:HG22	1.98	0.64
1:B:385:TYR:OH	1:C:71:ARG:HD3	1.98	0.64
1:A:151:ALA:O	1:A:154:VAL:HG12	1.97	0.63
1:C:367:THR:HB	1:D:291:GLU:HG2	1.78	0.63
1:F:211:LEU:O	1:F:215:ILE:HD12	1.98	0.63
1:C:392:ASP:HB2	1:C:412:ILE:O	1.98	0.63
1:C:335:LYS:HB3	1:D:108:VAL:HG11	1.79	0.63
1:C:138:VAL:HG12	1:C:179:GLY:HA2	1.81	0.63
1:E:212:LEU:HD22	1:E:307:ARG:NH2	2.11	0.63
1:E:212:LEU:HD21	1:E:304:PHE:HD1	1.63	0.63
1:E:92:VAL:HG21	1:E:132:LEU:HD13	1.79	0.63
1:E:212:LEU:CD2	1:E:307:ARG:HH21	2.11	0.63
1:C:357:ALA:O	1:C:361:LYS:HG2	1.99	0.62
1:E:258:ILE:HD11	1:E:290:VAL:HG23	1.81	0.62
1:E:303:GLU:CG	1:E:307:ARG:HH22	2.02	0.62
1:E:347:ASP:O	1:E:394:GLU:HG3	1.99	0.62
1:B:351:ARG:HD3	1:B:398:ILE:HG22	1.81	0.62
1:A:200:ARG:N	1:A:200:ARG:HD2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:O	1:B:189:ILE:HG12	2.00	0.62
1:E:159:GLU:HB2	1:E:235:PHE:CZ	2.35	0.62
1:A:148:LEU:HA	1:A:154:VAL:CG2	2.30	0.62
1:B:148:LEU:HB3	1:B:154:VAL:CG2	2.28	0.62
1:B:214:LEU:HD12	1:B:240:THR:HG21	1.81	0.62
1:E:403:ILE:HG13	1:E:404:ASP:H	1.65	0.62
1:D:365:ARG:O	1:D:366:LYS:HG2	2.00	0.62
1:C:162:ILE:HD11	1:C:214:LEU:HD11	1.81	0.62
1:E:104:THR:HG22	1:E:109:GLU:HB2	1.82	0.62
1:B:362:ALA:O	1:B:365:ARG:HG2	1.99	0.61
1:E:186:ILE:HD12	1:E:247:CYS:HB3	1.80	0.61
1:E:370:ARG:HG2	2:E:603:ADP:C5'	2.31	0.61
1:B:138:VAL:CG1	1:B:179:GLY:HA2	2.30	0.61
1:D:144:ASP:HB3	1:D:147:THR:CG2	2.30	0.61
1:F:211:LEU:HD12	1:F:214:LEU:HD21	1.82	0.61
1:D:386:ASP:HB3	1:E:68:HIS:NE2	2.15	0.61
1:F:403:ILE:HG13	1:F:404:ASP:N	2.16	0.61
1:C:212:LEU:HD11	1:C:307:ARG:HG3	1.83	0.61
1:B:212:LEU:HD13	1:B:304:PHE:HA	1.82	0.61
1:A:114:ASN:HD21	1:A:215:ILE:HG23	1.66	0.60
1:D:319:GLU:CD	1:D:319:GLU:H	2.04	0.60
1:F:147:THR:O	1:F:149:THR:HG23	2.01	0.60
1:B:340:LEU:HD21	1:C:94:ASN:ND2	2.16	0.60
1:F:301:ILE:HG12	1:F:304:PHE:HB2	1.83	0.60
1:C:258:ILE:HD13	1:C:286:LEU:O	2.02	0.60
1:E:166:LEU:HA	1:E:169:CYS:SG	2.41	0.60
1:D:158:VAL:O	1:D:161:ILE:HG12	2.02	0.59
1:C:161:ILE:HA	1:C:164:LYS:HE2	1.83	0.59
1:B:190:SER:HB2	1:B:299:GLY:HA3	1.85	0.59
1:D:399:ASP:O	1:D:403:ILE:HG13	2.03	0.59
1:F:64:LEU:N	1:F:65:PRO:HD3	2.17	0.59
1:E:296:ILE:CD1	1:E:305:ILE:HD12	2.32	0.59
1:F:173:VAL:O	1:F:177:GLN:HG3	2.03	0.59
1:D:81:GLN:O	1:D:85:LYS:HG3	2.02	0.59
1:A:156:GLU:O	1:A:159:GLU:HG2	2.02	0.59
1:E:151:ALA:HB3	1:E:154:VAL:HB	1.86	0.58
1:B:76:ASP:O	1:B:329:PRO:HA	2.03	0.58
1:D:177:GLN:OE1	1:D:239:ASP:HB2	2.04	0.58
1:B:259:SER:OG	1:B:286:LEU:HD21	2.04	0.58
1:D:293:GLU:HA	1:D:296:ILE:HG22	1.85	0.58
1:B:117:LEU:HD23	1:B:312:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HD3	1:B:191:ARG:NH1	2.18	0.58
1:B:217:GLY:HA2	1:B:240:THR:OG1	2.04	0.58
1:E:212:LEU:HD21	1:E:304:PHE:HA	1.85	0.58
1:E:211:LEU:O	1:E:215:ILE:HG13	2.03	0.58
1:E:292:PRO:O	1:E:296:ILE:HG12	2.03	0.58
1:E:212:LEU:HD13	1:E:307:ARG:NH2	2.19	0.58
1:A:154:VAL:O	1:A:158:VAL:HG23	2.03	0.58
1:C:175:LYS:HD3	1:C:178:ARG:NH1	2.18	0.58
1:F:73:HIS:CD2	1:F:135:LEU:HD13	2.38	0.58
1:E:213:LYS:HG2	1:E:214:LEU:N	2.19	0.57
1:F:186:ILE:HG21	1:F:247:CYS:HB3	1.85	0.57
1:E:79:ILE:H	2:E:603:ADP:HN62	1.52	0.57
1:A:71:ARG:HD3	1:F:385:TYR:OH	2.04	0.57
1:B:205:GLU:O	1:B:208:GLN:HB2	2.05	0.57
1:C:158:VAL:CG1	1:C:214:LEU:HB2	2.33	0.57
1:D:75:ASP:HA	1:D:85:LYS:NZ	2.20	0.57
1:C:365:ARG:HB2	1:C:367:THR:HG23	1.86	0.57
1:E:104:THR:HG21	1:E:110:LEU:N	2.19	0.57
1:F:138:VAL:HG13	1:F:179:GLY:HA2	1.86	0.57
1:A:356:ASP:O	1:A:360:LYS:HG3	2.05	0.57
1:C:212:LEU:HD21	1:C:303:GLU:HG2	1.86	0.57
1:E:398:ILE:HD12	1:E:401:SER:H	1.69	0.57
1:A:157:ASP:C	1:A:157:ASP:OD1	2.43	0.56
1:E:126:THR:HG22	1:E:182:TYR:CE2	2.39	0.56
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.87	0.56
1:E:153:TYR:HB3	1:F:202:VAL:HG11	1.85	0.56
1:D:370:ARG:CG	2:D:602:ADP:H5'1	2.35	0.56
1:C:292:PRO:O	1:C:296:ILE:HG13	2.06	0.56
1:E:210:ALA:HA	1:E:213:LYS:HD3	1.86	0.56
1:A:212:LEU:HD21	1:A:303:GLU:CG	2.35	0.56
1:D:114:ASN:HD21	1:D:215:ILE:HG23	1.69	0.56
1:E:186:ILE:O	1:E:189:ILE:HG12	2.05	0.56
1:E:209:GLN:HA	1:E:212:LEU:HD12	1.87	0.56
1:A:357:ALA:O	1:A:361:LYS:HG2	2.06	0.56
1:A:383:THR:OG1	1:A:409:PRO:HG3	2.06	0.56
1:E:367:THR:CG2	1:E:371:GLY:HA3	2.36	0.56
1:E:331:ASN:CG	1:F:109:GLU:HG2	2.26	0.56
1:F:130:GLU:HG2	1:F:140:PHE:CE2	2.41	0.56
1:F:146:THR:C	1:F:148:LEU:HD23	2.26	0.56
1:F:200:ARG:HG3	1:F:201:ASP:N	2.21	0.56
1:F:293:GLU:O	1:F:297:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:ARG:HG2	2:D:602:ADP:H5'1	1.88	0.55
1:D:319:GLU:HG3	1:D:363:MET:SD	2.47	0.55
1:E:177:GLN:HA	1:E:243:ILE:HG22	1.88	0.55
1:C:189:ILE:O	1:C:204:GLY:HA3	2.06	0.55
1:F:301:ILE:HG13	1:F:304:PHE:H	1.71	0.55
1:A:154:VAL:CA	1:A:157:ASP:HB3	2.25	0.55
1:E:189:ILE:HB	1:E:207:VAL:HG21	1.89	0.55
1:D:254:LEU:O	1:D:258:ILE:HG13	2.06	0.55
1:E:210:ALA:O	1:E:213:LYS:HG2	2.07	0.55
1:C:95:HIS:CD2	1:C:244:LEU:HD13	2.42	0.55
1:C:258:ILE:HD11	1:C:289:GLN:C	2.27	0.55
1:D:251:PHE:HB3	1:D:254:LEU:HB2	1.89	0.55
1:F:114:ASN:HD21	1:F:215:ILE:HG21	1.71	0.55
1:D:215:ILE:HG21	1:D:307:ARG:HB3	1.89	0.54
1:B:98:ARG:HG3	1:B:110:LEU:HD12	1.89	0.54
1:E:322:LEU:HD23	1:E:372:LEU:HD21	1.89	0.54
1:D:160:ASN:O	1:D:164:LYS:HG3	2.07	0.54
1:D:92:VAL:HG11	1:D:136:LEU:HD11	1.89	0.54
1:A:307:ARG:O	1:A:309:PRO:HD3	2.07	0.54
1:B:392:ASP:OD2	1:B:411:LEU:HG	2.07	0.54
1:D:148:LEU:HD21	1:D:158:VAL:CG1	2.23	0.54
1:F:387:LEU:HB3	1:F:388:PRO:HD3	1.89	0.54
1:A:151:ALA:HB1	1:A:153:TYR:CD1	2.42	0.54
1:B:307:ARG:C	1:B:309:PRO:HD3	2.28	0.54
1:B:386:ASP:HA	1:C:68:HIS:CD2	2.43	0.54
1:E:243:ILE:HD11	1:E:245:PHE:CZ	2.43	0.54
1:F:138:VAL:CG1	1:F:179:GLY:HA2	2.37	0.54
1:A:344:GLU:HG3	1:A:387:LEU:HD21	1.89	0.53
1:A:98:ARG:HD2	1:A:110:LEU:CB	2.38	0.53
1:D:351:ARG:HG3	1:D:398:ILE:HG22	1.90	0.53
1:E:148:LEU:HA	1:E:154:VAL:CG2	2.28	0.53
1:E:254:LEU:O	1:E:258:ILE:HG12	2.08	0.53
1:E:235:PHE:CE1	1:E:236:LEU:HD22	2.44	0.53
1:B:208:GLN:OE1	1:B:301:ILE:HG23	2.09	0.53
1:F:169:CYS:SG	1:F:175:LYS:HB2	2.48	0.53
1:C:392:ASP:HB3	1:C:413:TYR:CD2	2.43	0.53
1:E:358:ILE:HD13	1:E:376:VAL:HG22	1.90	0.53
1:A:140:PHE:CE2	1:A:142:MET:HG3	2.44	0.53
1:E:104:THR:HG21	1:E:109:GLU:H	1.72	0.53
1:F:145:ALA:HB3	1:F:185:GLN:HB2	1.90	0.53
1:F:220:ALA:HA	1:F:237:GLN:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:CB	1:A:108:VAL:HB	2.40	0.52
1:A:154:VAL:O	1:A:158:VAL:N	2.42	0.52
1:A:172:ASP:OD1	1:A:174:GLN:HG2	2.09	0.52
1:D:144:ASP:OD2	1:D:146:THR:OG1	2.27	0.52
1:E:104:THR:HG21	1:E:109:GLU:CA	2.38	0.52
1:E:331:ASN:OD1	1:F:109:GLU:HG2	2.09	0.52
1:F:116:LEU:HD12	1:F:247:CYS:O	2.09	0.52
1:D:354:ALA:O	1:D:358:ILE:HG13	2.10	0.52
1:A:212:LEU:HD21	1:A:303:GLU:HG3	1.92	0.52
1:E:104:THR:HG21	1:E:110:LEU:H	1.74	0.52
1:E:208:GLN:O	1:E:212:LEU:HG	2.10	0.52
1:F:234:GLU:HG2	1:F:235:PHE:CD2	2.44	0.52
1:C:161:ILE:HD11	1:C:214:LEU:CD2	2.39	0.52
1:A:109:GLU:HG3	1:F:330:LYS:O	2.10	0.52
1:E:95:HIS:NE2	1:E:99:LEU:HD11	2.24	0.52
1:A:254:LEU:O	1:A:257:VAL:HG12	2.10	0.52
1:B:154:VAL:HG21	1:B:207:VAL:HG22	1.91	0.52
1:C:255:ASP:O	1:C:258:ILE:HG22	2.10	0.52
1:B:386:ASP:HB3	1:C:68:HIS:NE2	2.25	0.52
1:D:145:ALA:HB3	1:D:185:GLN:O	2.08	0.52
1:D:293:GLU:O	1:D:296:ILE:HG22	2.09	0.52
1:A:358:ILE:HD13	1:A:376:VAL:HG22	1.91	0.52
1:B:232:GLN:O	1:B:233:GLN:HG3	2.09	0.52
1:C:406:GLN:HG3	1:C:407:SER:N	2.25	0.52
1:D:96:TYR:CE1	1:D:136:LEU:HD13	2.45	0.52
1:C:404:ASP:HB3	1:C:406:GLN:HG2	1.91	0.52
1:D:127:LEU:HD22	2:D:602:ADP:H2'	1.92	0.52
1:A:149:THR:CA	1:A:207:VAL:HG21	2.39	0.52
1:E:138:VAL:CG1	1:E:179:GLY:HA2	2.39	0.52
1:E:148:LEU:HB3	1:E:154:VAL:HG21	1.92	0.52
1:F:110:LEU:N	1:F:110:LEU:HD12	2.25	0.52
1:D:282:SER:O	1:D:286:LEU:HG	2.10	0.52
1:E:138:VAL:HG13	1:E:179:GLY:HA2	1.92	0.52
1:F:177:GLN:HG2	1:F:238:VAL:HG13	1.90	0.51
1:F:319:GLU:O	1:F:323:ILE:HG13	2.10	0.51
1:B:167:GLN:NE2	1:C:218:THR:HG22	2.25	0.51
1:C:291:GLU:CG	1:C:292:PRO:HD2	2.39	0.51
1:C:351:ARG:HG3	1:C:398:ILE:HG22	1.92	0.51
1:D:387:LEU:HB3	1:D:388:PRO:HD3	1.91	0.51
1:B:135:LEU:HD12	1:B:136:LEU:HG	1.91	0.51
1:E:388:PRO:HG2	1:F:67:PRO:CD	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:SER:O	1:A:196:PRO:HD3	2.10	0.51
1:E:403:ILE:HG13	1:E:404:ASP:N	2.23	0.51
1:A:91:ALA:HB2	1:A:310:VAL:HG11	1.91	0.51
1:D:205:GLU:O	1:D:208:GLN:HB2	2.11	0.51
1:D:344:GLU:OE2	1:D:388:PRO:HG3	2.11	0.51
1:E:79:ILE:N	2:E:603:ADP:HN62	2.08	0.51
1:E:144:ASP:OD2	1:F:302:PRO:HD3	2.11	0.51
1:E:325:ILE:HG23	2:E:603:ADP:N3	2.26	0.51
1:A:78:VAL:HG21	1:A:128:LEU:HD23	1.93	0.51
1:C:240:THR:O	1:C:243:ILE:HG12	2.10	0.51
1:E:148:LEU:CB	1:E:154:VAL:HG21	2.40	0.51
1:B:399:ASP:O	1:B:403:ILE:HG22	2.11	0.51
1:E:251:PHE:HB3	1:E:254:LEU:HB3	1.92	0.51
1:E:212:LEU:HD11	1:E:301:ILE:HD11	1.93	0.51
1:C:398:ILE:HG13	1:C:400:GLU:HG2	1.92	0.51
1:D:104:THR:HG22	1:D:110:LEU:HB3	1.92	0.51
1:E:212:LEU:CD2	1:E:304:PHE:HD1	2.22	0.51
1:F:144:ASP:O	1:F:147:THR:HG22	2.10	0.51
1:F:81:GLN:HE22	1:F:316:GLU:N	2.02	0.51
1:B:387:LEU:HB3	1:B:388:PRO:HD3	1.91	0.50
1:A:209:GLN:O	1:A:212:LEU:HB3	2.11	0.50
1:B:177:GLN:HB3	1:B:242:LYS:HB2	1.92	0.50
1:A:101:ASN:HD22	1:F:343:LEU:HD22	1.76	0.50
1:C:336:GLN:O	1:C:340:LEU:HD13	2.11	0.50
1:E:189:ILE:HD12	1:E:207:VAL:HG23	1.94	0.50
1:F:287:LEU:HD23	1:F:313:THR:HB	1.94	0.50
1:E:160:ASN:OD1	1:E:160:ASN:O	2.30	0.50
1:A:108:VAL:HG12	1:A:109:GLU:N	2.26	0.50
1:E:79:ILE:H	2:E:603:ADP:N6	2.09	0.50
1:F:186:ILE:HG13	1:F:187:ASP:N	2.25	0.50
1:F:152:GLY:O	1:F:154:VAL:CG2	2.49	0.50
1:C:307:ARG:O	1:C:309:PRO:HD3	2.12	0.50
1:D:296:ILE:HD12	1:D:300:LEU:O	2.12	0.50
1:E:258:ILE:O	1:E:262:VAL:HG22	2.11	0.50
1:F:403:ILE:HG13	1:F:404:ASP:H	1.75	0.50
1:E:99:LEU:HD13	1:E:242:LYS:HE3	1.93	0.50
1:F:155:GLY:O	1:F:158:VAL:HG22	2.11	0.50
1:D:187:ASP:OD1	1:D:187:ASP:N	2.45	0.49
1:A:391:GLU:N	1:A:391:GLU:CD	2.66	0.49
1:D:307:ARG:O	1:D:309:PRO:HD3	2.12	0.49
1:E:343:LEU:HD22	1:F:101:ASN:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:ASN:O	1:F:164:LYS:HG3	2.12	0.49
1:A:96:TYR:O	1:A:100:ARG:HG3	2.12	0.49
1:E:293:GLU:H	1:E:293:GLU:CD	2.16	0.49
1:F:354:ALA:O	1:F:358:ILE:HG13	2.11	0.49
1:B:258:ILE:O	1:B:261:ARG:HG2	2.12	0.49
1:E:257:VAL:HA	1:E:260:HIS:HD2	1.77	0.49
1:A:148:LEU:O	1:A:154:VAL:HG21	2.13	0.49
1:A:141:THR:CG2	1:A:181:VAL:HG22	2.43	0.49
1:E:370:ARG:HD3	2:E:603:ADP:H4'	1.95	0.49
1:F:149:THR:C	1:F:157:ASP:CB	2.81	0.49
1:B:170:ASP:O	1:B:171:TYR:HB2	2.12	0.49
1:C:199:THR:HG22	1:C:201:ASP:H	1.78	0.49
1:D:307:ARG:C	1:D:309:PRO:HD3	2.33	0.49
1:D:96:TYR:O	1:D:100:ARG:HG3	2.12	0.49
1:F:236:LEU:CD2	1:F:236:LEU:H	2.26	0.49
1:A:119:GLY:O	1:A:250:ALA:HA	2.12	0.49
1:E:296:ILE:HD13	1:E:305:ILE:HD12	1.93	0.49
1:F:81:GLN:HE22	1:F:315:ASN:H	1.60	0.49
1:C:386:ASP:HB3	1:D:68:HIS:NE2	2.27	0.49
1:E:99:LEU:HD22	1:E:242:LYS:HG3	1.94	0.49
1:F:301:ILE:HG12	1:F:304:PHE:CB	2.43	0.49
1:A:109:GLU:HG3	1:F:331:ASN:HA	1.94	0.48
1:C:315:ASN:HD22	1:C:315:ASN:N	2.03	0.48
1:D:64:LEU:CD1	1:D:65:PRO:HD2	2.42	0.48
1:E:208:GLN:OE1	1:E:301:ILE:HG12	2.12	0.48
1:F:301:ILE:CG1	1:F:304:PHE:HB2	2.42	0.48
1:D:222:VAL:N	1:D:223:PRO:CD	2.76	0.48
1:E:177:GLN:HB2	1:E:242:LYS:HD3	1.96	0.48
1:F:153:TYR:O	1:F:154:VAL:HB	2.12	0.48
1:F:221:ALA:O	1:F:223:PRO:HD3	2.13	0.48
1:E:163:GLN:HA	1:E:166:LEU:HG	1.95	0.48
1:E:173:VAL:HG21	1:E:237:GLN:OE1	2.13	0.48
1:E:95:HIS:O	1:E:99:LEU:HG	2.13	0.48
1:F:202:VAL:HA	1:F:205:GLU:HG3	1.95	0.48
1:C:243:ILE:HD11	1:C:245:PHE:CZ	2.47	0.48
1:C:117:LEU:HD23	1:C:312:ALA:HB3	1.95	0.48
1:D:169:CYS:O	1:D:170:ASP:HB2	2.14	0.48
1:E:212:LEU:HD13	1:E:307:ARG:HH21	1.79	0.48
1:D:164:LYS:NZ	1:E:209:GLN:HE22	2.10	0.48
1:D:251:PHE:HB3	1:D:254:LEU:CB	2.44	0.48
1:F:254:LEU:O	1:F:258:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:O	1:A:237:GLN:HG2	2.14	0.48
1:A:243:ILE:HD11	1:A:245:PHE:CE2	2.49	0.48
1:C:403:ILE:HG23	1:C:404:ASP:N	2.29	0.48
1:D:157:ASP:OD1	1:D:157:ASP:C	2.52	0.48
1:D:78:VAL:HG13	2:D:602:ADP:N6	2.29	0.48
1:C:400:GLU:HB2	1:C:406:GLN:NE2	2.28	0.48
1:B:361:LYS:NZ	1:B:403:ILE:HA	2.29	0.48
1:A:125:LYS:HG2	1:A:314:LEU:HD22	1.95	0.47
1:B:370:ARG:CG	2:B:601:ADP:H5'1	2.45	0.47
1:D:73:HIS:HB3	1:D:135:LEU:HD22	1.97	0.47
1:F:172:ASP:OD2	1:F:175:LYS:HG3	2.14	0.47
1:D:346:VAL:HG21	1:D:387:LEU:HD11	1.94	0.47
1:B:169:CYS:O	1:B:170:ASP:HB2	2.14	0.47
1:B:346:VAL:HG21	1:B:387:LEU:HD11	1.97	0.47
1:B:142:MET:SD	1:C:303:GLU:HB2	2.54	0.47
1:E:343:LEU:HD13	1:F:101:ASN:HD22	1.78	0.47
1:A:150:GLU:CB	1:B:191:ARG:HH22	2.27	0.47
1:F:163:GLN:O	1:F:167:GLN:HG2	2.14	0.47
1:F:212:LEU:HD21	1:F:303:GLU:HG2	1.97	0.47
1:C:296:ILE:HG12	1:C:305:ILE:HD12	1.97	0.47
1:E:102:GLY:O	1:E:103:ASP:C	2.52	0.47
1:F:78:VAL:HG23	1:F:127:LEU:HD23	1.96	0.47
1:D:169:CYS:SG	1:D:175:LYS:CB	3.03	0.47
1:E:212:LEU:HD22	1:E:307:ARG:HE	1.80	0.47
1:E:214:LEU:O	1:E:240:THR:HB	2.15	0.47
1:B:347:ASP:O	1:B:394:GLU:HB2	2.15	0.47
1:C:149:THR:O	1:C:202:VAL:HB	2.15	0.47
1:C:261:ARG:HD3	1:C:294:ASP:OD1	2.15	0.47
1:C:190:SER:HB2	1:C:299:GLY:HA3	1.97	0.47
1:F:214:LEU:C	1:F:214:LEU:HD12	2.35	0.47
1:A:387:LEU:HB3	1:A:388:PRO:HD3	1.96	0.47
1:E:116:LEU:HD13	1:E:308:LEU:HD23	1.97	0.47
1:A:151:ALA:HB3	1:A:154:VAL:CB	2.33	0.47
1:C:70:ILE:O	1:C:74:LEU:HG	2.15	0.47
1:D:144:ASP:O	1:D:147:THR:CG2	2.54	0.47
1:D:332:ALA:O	1:D:336:GLN:HG3	2.15	0.46
1:E:319:GLU:OE2	1:E:360:LYS:HE2	2.16	0.46
1:B:301:ILE:HG12	1:B:304:PHE:HB2	1.95	0.46
1:C:138:VAL:HG11	1:C:178:ARG:O	2.15	0.46
1:D:165:LEU:O	1:D:165:LEU:HD23	2.15	0.46
1:E:104:THR:CG2	1:E:110:LEU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ILE:HA	1:F:164:LYS:HE2	1.97	0.46
1:C:383:THR:O	1:C:387:LEU:HB2	2.14	0.46
1:E:190:SER:OG	1:E:299:GLY:HA3	2.15	0.46
1:F:86:LYS:O	1:F:90:VAL:HG23	2.14	0.46
1:A:160:ASN:HA	1:A:163:GLN:HG2	1.96	0.46
1:A:217:GLY:HA3	1:A:241:SER:OG	2.16	0.46
1:B:230:HIS:N	1:B:231:PRO:CD	2.77	0.46
1:C:317:LEU:HD21	1:C:368:GLY:HA2	1.98	0.46
1:D:114:ASN:H	1:D:309:PRO:HD2	1.79	0.46
1:D:148:LEU:CD2	1:D:158:VAL:HG12	2.25	0.46
1:D:166:LEU:HD22	1:D:171:TYR:HA	1.96	0.46
1:D:90:VAL:HG12	1:D:94:ASN:ND2	2.29	0.46
1:A:151:ALA:CB	1:A:153:TYR:CZ	2.97	0.46
1:C:403:ILE:CG2	1:C:404:ASP:N	2.78	0.46
1:E:163:GLN:O	1:E:167:GLN:HG3	2.16	0.46
1:E:370:ARG:HA	1:E:370:ARG:HD3	1.76	0.46
1:F:170:ASP:O	1:F:171:TYR:HB2	2.14	0.46
1:A:182:TYR:HA	1:A:246:ILE:O	2.16	0.46
1:B:162:ILE:HD11	1:B:240:THR:HG22	1.98	0.46
1:C:169:CYS:O	1:C:170:ASP:HB3	2.16	0.46
1:D:340:LEU:HD21	1:E:94:ASN:ND2	2.31	0.46
1:A:79:ILE:H	2:A:600:ADP:HN62	1.64	0.46
1:C:158:VAL:HG12	1:C:214:LEU:HD13	1.98	0.46
1:C:174:GLN:HE21	1:C:178:ARG:HH11	1.62	0.46
1:E:149:THR:HB	1:E:189:ILE:HG22	1.96	0.46
1:F:114:ASN:HD22	1:F:307:ARG:HG3	1.80	0.46
1:F:117:LEU:HD23	1:F:312:ALA:HB3	1.96	0.46
1:F:205:GLU:O	1:F:208:GLN:HG2	2.16	0.46
1:A:108:VAL:HG12	1:A:109:GLU:H	1.81	0.46
1:B:170:ASP:OD2	1:C:219:VAL:HG13	2.15	0.46
1:B:371:GLY:O	1:B:375:ILE:HG13	2.16	0.46
1:D:161:ILE:HA	1:D:164:LYS:HD2	1.98	0.46
1:E:177:GLN:O	1:E:242:LYS:HG2	2.16	0.46
1:E:212:LEU:CD2	1:E:304:PHE:HA	2.45	0.46
1:A:151:ALA:CB	1:A:153:TYR:CE1	2.99	0.46
1:A:112:LYS:CE	1:A:307:ARG:HE	2.27	0.46
1:A:166:LEU:HD11	1:A:238:VAL:HG21	1.98	0.45
1:A:401:SER:O	1:A:405:GLY:HA2	2.15	0.45
1:C:92:VAL:CG1	1:C:136:LEU:HD11	2.46	0.45
1:F:124:GLY:O	1:F:128:LEU:HG	2.16	0.45
1:F:258:ILE:HG12	1:F:294:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:ASN:HB2	1:F:307:ARG:O	2.15	0.45
1:B:151:ALA:O	1:B:154:VAL:HG12	2.16	0.45
1:E:157:ASP:O	1:E:157:ASP:OD1	2.33	0.45
1:F:359:ALA:O	1:F:363:MET:HG3	2.15	0.45
1:A:261:ARG:NH2	1:A:291:GLU:HG3	2.31	0.45
1:C:257:VAL:HG13	1:C:297:LYS:HD3	1.99	0.45
1:D:73:HIS:HB3	1:D:135:LEU:CD2	2.47	0.45
1:B:338:GLN:O	1:B:342:ASN:HB2	2.17	0.45
1:C:149:THR:HA	1:C:207:VAL:HG21	1.98	0.45
1:F:283:GLU:O	1:F:287:LEU:HD13	2.17	0.45
1:F:73:HIS:HE1	1:F:131:THR:HG23	1.82	0.45
1:B:261:ARG:HD2	1:B:294:ASP:OD1	2.16	0.45
1:E:391:GLU:O	1:E:391:GLU:HG2	2.17	0.45
1:B:148:LEU:O	1:B:154:VAL:HB	2.16	0.45
1:B:205:GLU:HA	1:B:208:GLN:CG	2.42	0.45
1:C:114:ASN:HB2	1:C:307:ARG:O	2.16	0.45
1:C:78:VAL:HG22	1:C:127:LEU:HD23	1.98	0.45
1:E:371:GLY:O	1:E:375:ILE:HG13	2.17	0.45
1:E:114:ASN:ND2	1:E:215:ILE:HD13	2.31	0.45
1:E:212:LEU:HD21	1:E:304:PHE:CD1	2.46	0.45
1:F:156:GLU:HA	1:F:159:GLU:HG2	1.98	0.45
1:A:354:ALA:O	1:A:358:ILE:HG13	2.17	0.45
1:F:73:HIS:HB3	1:F:135:LEU:HD22	1.99	0.45
1:C:114:ASN:HB3	1:C:308:LEU:HD23	1.98	0.45
1:F:184:ASP:C	1:F:185:GLN:HG2	2.37	0.45
1:F:81:GLN:NE2	1:F:314:LEU:HB3	2.31	0.45
1:A:195:ASN:N	1:A:196:PRO:CD	2.80	0.45
1:B:354:ALA:O	1:B:358:ILE:HG13	2.17	0.45
1:D:66:THR:CG2	1:D:69:GLU:HB2	2.47	0.45
1:E:327:LYS:HD3	1:E:355:LEU:HD13	1.99	0.45
1:F:296:ILE:HD11	1:F:302:PRO:HA	1.97	0.45
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.82	0.44
1:B:347:ASP:HB3	1:B:394:GLU:HB2	1.98	0.44
1:C:145:ALA:HB1	1:C:189:ILE:CG2	2.47	0.44
1:C:317:LEU:HB2	1:C:363:MET:HG2	1.99	0.44
1:E:251:PHE:HB3	1:E:254:LEU:CB	2.47	0.44
1:E:75:ASP:HA	1:E:85:LYS:HZ3	1.82	0.44
1:B:173:VAL:HG13	1:B:238:VAL:HB	1.98	0.44
1:D:83:GLN:O	1:D:87:VAL:HG23	2.17	0.44
1:E:151:ALA:C	1:E:154:VAL:HG12	2.37	0.44
1:E:172:ASP:O	1:E:173:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ALA:CB	1:B:140:PHE:HB2	2.47	0.44
1:B:208:GLN:O	1:B:212:LEU:HB2	2.17	0.44
1:B:212:LEU:HD21	1:B:303:GLU:CG	2.48	0.44
1:E:104:THR:HG21	1:E:109:GLU:HB2	1.98	0.44
1:E:131:THR:O	1:E:135:LEU:HG	2.18	0.44
1:E:163:GLN:NE2	1:E:166:LEU:HD11	2.33	0.44
1:E:387:LEU:N	1:E:388:PRO:CD	2.80	0.44
1:F:254:LEU:HA	1:F:257:VAL:HG12	1.99	0.44
1:F:71:ARG:NH2	1:F:82:GLU:OE1	2.50	0.44
1:A:301:ILE:HG13	1:A:304:PHE:H	1.81	0.44
1:B:232:GLN:C	1:B:233:GLN:HG3	2.37	0.44
1:D:117:LEU:HD23	1:D:312:ALA:HB3	1.98	0.44
1:A:151:ALA:HB1	1:A:153:TYR:CG	2.53	0.44
1:A:148:LEU:CA	1:A:154:VAL:HG21	2.39	0.44
1:E:386:ASP:HB3	1:F:68:HIS:CE1	2.51	0.44
1:F:177:GLN:CG	1:F:238:VAL:HG13	2.47	0.44
1:D:190:SER:OG	1:D:299:GLY:HA3	2.17	0.44
1:D:75:ASP:HA	1:D:85:LYS:HZ3	1.81	0.44
1:E:114:ASN:HB2	1:E:307:ARG:O	2.17	0.44
1:A:307:ARG:C	1:A:309:PRO:HD3	2.38	0.43
1:D:79:ILE:HD12	1:D:325:ILE:HA	2.00	0.43
1:E:110:LEU:CB	1:E:112:LYS:HE2	2.48	0.43
1:C:356:ASP:O	1:C:360:LYS:HG3	2.17	0.43
1:C:317:LEU:CD2	1:C:368:GLY:HA2	2.49	0.43
1:D:202:VAL:C	1:D:204:GLY:N	2.71	0.43
1:D:212:LEU:HD23	1:D:212:LEU:C	2.38	0.43
1:B:365:ARG:HG3	1:B:367:THR:CG2	2.47	0.43
1:D:114:ASN:HB2	1:D:307:ARG:O	2.18	0.43
1:E:344:GLU:OE2	1:E:388:PRO:HG3	2.18	0.43
1:F:361:LYS:HD3	1:F:365:ARG:NH2	2.34	0.43
1:B:324:GLN:HG3	1:B:328:GLU:OE2	2.18	0.43
1:D:204:GLY:O	1:D:207:VAL:N	2.50	0.43
1:E:258:ILE:HD12	1:E:290:VAL:HA	2.00	0.43
1:A:254:LEU:O	1:A:258:ILE:HG13	2.19	0.43
1:B:296:ILE:HD12	1:B:302:PRO:HG3	2.01	0.43
1:C:64:LEU:HD22	1:C:100:ARG:HD2	2.00	0.43
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.83	0.43
1:C:136:LEU:HB3	1:C:138:VAL:HG23	2.00	0.43
1:D:222:VAL:CG1	1:D:223:PRO:HD3	2.49	0.43
1:D:357:ALA:HB1	1:D:403:ILE:CG1	2.42	0.43
1:D:393:VAL:CB	1:D:414:GLY:HA3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:VAL:O	1:E:85:LYS:NZ	2.51	0.43
1:F:220:ALA:HA	1:F:237:GLN:CD	2.39	0.43
1:B:232:GLN:HB3	1:B:235:PHE:HB3	2.00	0.43
1:C:195:ASN:HA	1:C:196:PRO:HD2	1.83	0.43
1:C:392:ASP:N	1:C:392:ASP:OD1	2.48	0.43
1:B:388:PRO:HG2	1:C:67:PRO:CD	2.49	0.43
1:F:201:ASP:OD1	1:F:202:VAL:HG23	2.19	0.43
1:A:149:THR:N	1:A:207:VAL:HG21	2.33	0.43
1:D:88:LEU:HD23	1:D:115:ILE:HD13	2.01	0.43
1:D:175:LYS:HA	1:D:178:ARG:HD2	2.00	0.43
1:E:155:GLY:O	1:E:158:VAL:HB	2.19	0.43
1:E:295:LEU:HB2	1:E:305:ILE:HD13	2.00	0.43
1:A:86:LYS:HG3	1:F:385:TYR:CD1	2.54	0.43
1:D:326:LEU:O	1:D:332:ALA:HB1	2.18	0.43
1:D:386:ASP:HA	1:E:68:HIS:CD2	2.53	0.43
1:E:343:LEU:HD22	1:F:101:ASN:ND2	2.33	0.43
1:F:146:THR:HG23	1:F:185:GLN:HB3	2.01	0.43
1:A:186:ILE:O	1:A:189:ILE:HG12	2.19	0.43
1:D:167:GLN:CG	1:D:168:LYS:N	2.81	0.43
1:C:367:THR:CB	1:D:291:GLU:HG2	2.47	0.43
1:E:157:ASP:C	1:E:160:ASN:H	2.22	0.43
1:D:173:VAL:O	1:D:177:GLN:HG2	2.19	0.42
1:D:208:GLN:O	1:D:212:LEU:N	2.52	0.42
1:D:221:ALA:CB	1:D:223:PRO:HD2	2.49	0.42
1:F:156:GLU:O	1:F:159:GLU:HG2	2.19	0.42
1:F:142:MET:HG3	1:F:182:TYR:HD2	1.84	0.42
1:F:95:HIS:NE2	1:F:244:LEU:HB2	2.34	0.42
1:B:118:ILE:O	1:B:313:THR:HA	2.19	0.42
1:C:116:LEU:HD12	1:C:247:CYS:O	2.19	0.42
1:D:160:ASN:O	1:D:163:GLN:HB3	2.19	0.42
1:D:125:LYS:HG2	1:D:314:LEU:CD1	2.49	0.42
1:E:160:ASN:HA	1:E:163:GLN:HB3	2.01	0.42
1:F:184:ASP:OD1	1:F:185:GLN:N	2.52	0.42
1:F:406:GLN:HG3	1:F:407:SER:N	2.35	0.42
1:A:92:VAL:HG21	1:A:132:LEU:HD22	2.02	0.42
1:B:75:ASP:OD1	1:B:85:LYS:HE2	2.18	0.42
1:C:347:ASP:O	1:C:394:GLU:HB2	2.19	0.42
1:A:131:THR:O	1:A:135:LEU:HG	2.20	0.42
1:A:398:ILE:HG13	1:A:400:GLU:N	2.34	0.42
1:D:133:ALA:CB	1:D:140:PHE:HB2	2.49	0.42
1:E:154:VAL:O	1:E:154:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:VAL:O	1:E:158:VAL:N	2.52	0.42
1:F:186:ILE:HD13	1:F:247:CYS:HB3	2.02	0.42
1:A:163:GLN:HG3	1:A:164:LYS:N	2.35	0.42
1:B:235:PHE:O	1:B:238:VAL:HG12	2.18	0.42
1:E:103:ASP:C	1:E:104:THR:HG23	2.40	0.42
1:B:361:LYS:HB2	1:B:361:LYS:HE3	1.89	0.42
1:B:99:LEU:HD22	1:B:242:LYS:HD2	2.01	0.42
1:D:221:ALA:HB3	1:D:223:PRO:HD2	2.02	0.42
1:A:86:LYS:HD2	1:F:381:LEU:CD1	2.50	0.42
1:D:189:ILE:CD1	1:D:208:GLN:HG3	2.49	0.42
1:D:79:ILE:HD11	1:D:329:PRO:HD3	2.02	0.42
1:E:326:LEU:O	1:E:332:ALA:HB1	2.20	0.42
1:A:141:THR:HB	1:A:168:LYS:HE3	2.02	0.42
1:C:360:LYS:HA	1:C:363:MET:CE	2.50	0.42
1:D:179:GLY:O	1:D:243:ILE:HG23	2.20	0.42
1:E:151:ALA:O	1:E:154:VAL:CG1	2.58	0.42
1:B:403:ILE:HG23	1:B:404:ASP:N	2.34	0.42
1:C:135:LEU:C	1:C:135:LEU:HD12	2.39	0.42
1:F:341:PHE:CD1	1:F:348:LEU:HD22	2.54	0.42
1:A:369:ALA:HA	1:A:372:LEU:HG	2.02	0.41
1:C:371:GLY:O	1:C:375:ILE:HG13	2.20	0.41
1:E:104:THR:OG1	1:E:107:GLY:N	2.53	0.41
1:E:114:ASN:HD21	1:E:215:ILE:HD13	1.84	0.41
1:F:154:VAL:HG12	1:F:154:VAL:O	2.20	0.41
1:A:162:ILE:O	1:A:166:LEU:HD13	2.20	0.41
1:C:135:LEU:HD12	1:C:136:LEU:N	2.34	0.41
1:D:66:THR:HG22	1:D:69:GLU:HB2	2.01	0.41
1:B:166:LEU:HD22	1:B:171:TYR:HA	2.01	0.41
1:D:189:ILE:HG12	1:D:208:GLN:HE21	1.86	0.41
1:B:295:LEU:HB2	1:B:305:ILE:HD13	2.02	0.41
1:D:380:LEU:O	1:D:384:MET:HG3	2.20	0.41
1:F:105:SER:O	1:F:106:ASN:HB2	2.21	0.41
1:F:347:ASP:O	1:F:394:GLU:HB2	2.20	0.41
1:A:177:GLN:HA	1:A:243:ILE:HG22	2.02	0.41
1:A:391:GLU:HG2	1:A:391:GLU:O	2.20	0.41
1:C:199:THR:HG22	1:C:201:ASP:N	2.35	0.41
1:E:254:LEU:HA	1:E:257:VAL:HG12	2.02	0.41
1:A:208:GLN:O	1:A:212:LEU:HB2	2.20	0.41
1:C:346:VAL:HG21	1:C:387:LEU:HD11	2.03	0.41
1:D:173:VAL:HG13	1:D:237:GLN:O	2.21	0.41
1:A:371:GLY:O	1:A:375:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LEU:HD22	1:D:304:PHE:HD2	1.85	0.41
1:E:159:GLU:HB2	1:E:235:PHE:CE1	2.56	0.41
1:E:76:ASP:O	1:E:329:PRO:HA	2.21	0.41
1:A:386:ASP:HB3	1:B:68:HIS:NE2	2.35	0.41
1:E:144:ASP:HB3	1:E:147:THR:HG23	2.02	0.41
1:E:173:VAL:HG21	1:E:237:GLN:HB3	2.03	0.41
1:E:382:ASP:O	1:E:385:TYR:HB3	2.21	0.41
1:F:146:THR:HG23	1:F:185:GLN:CB	2.51	0.41
1:A:151:ALA:HB2	1:A:153:TYR:CE1	2.56	0.41
1:A:251:PHE:HB3	1:A:254:LEU:CB	2.51	0.41
1:B:216:GLU:CD	1:B:307:ARG:HD2	2.41	0.41
1:B:212:LEU:HD21	1:B:303:GLU:HG3	2.03	0.41
1:B:369:ALA:HB3	2:B:601:ADP:C8	2.55	0.41
1:E:363:MET:HB2	1:E:363:MET:HE2	1.86	0.41
1:E:346:VAL:HG21	1:E:387:LEU:HD11	2.03	0.41
1:F:114:ASN:HB3	1:F:308:LEU:CD1	2.48	0.41
1:A:396:VAL:HB	1:A:410:LEU:HB3	2.03	0.41
1:B:207:VAL:HG12	1:B:211:LEU:HD22	2.03	0.41
1:B:301:ILE:HG13	1:B:304:PHE:H	1.84	0.41
1:B:370:ARG:HG3	2:B:601:ADP:H5'1	2.02	0.41
1:C:380:LEU:O	1:C:384:MET:HG3	2.21	0.41
1:D:202:VAL:O	1:D:202:VAL:HG12	2.21	0.41
1:A:296:ILE:HD11	1:A:302:PRO:HA	2.03	0.41
1:C:250:ALA:O	5:C:803:HOH:O	2.22	0.41
1:C:391:GLU:O	1:C:391:GLU:HG2	2.21	0.41
1:E:146:THR:O	1:E:149:THR:HG22	2.21	0.41
1:E:173:VAL:CG1	1:E:238:VAL:HB	2.38	0.41
1:B:151:ALA:HB1	1:B:153:TYR:CE1	2.57	0.40
1:C:333:LEU:HD22	1:C:337:TYR:HE1	1.86	0.40
1:E:104:THR:OG1	1:E:107:GLY:CA	2.69	0.40
1:E:141:THR:CG2	1:E:181:VAL:HG22	2.51	0.40
1:F:153:TYR:O	1:F:154:VAL:CB	2.68	0.40
1:D:101:ASN:OD1	1:D:101:ASN:C	2.59	0.40
1:D:116:LEU:HD12	1:D:247:CYS:O	2.21	0.40
1:D:254:LEU:HG	1:D:258:ILE:HD11	2.02	0.40
1:C:367:THR:CG2	1:D:291:GLU:HG2	2.51	0.40
1:E:329:PRO:CG	2:E:603:ADP:H2	2.34	0.40
1:F:104:THR:O	1:F:105:SER:HB2	2.21	0.40
1:A:261:ARG:HH21	1:F:365:ARG:HB3	1.86	0.40
1:B:251:PHE:HB3	1:B:254:LEU:HB2	2.03	0.40
1:B:321:ALA:O	1:B:325:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:NE2	1:C:316:GLU:H	2.15	0.40
1:C:404:ASP:C	1:C:406:GLN:N	2.74	0.40
1:D:206:GLY:O	1:D:209:GLN:HB3	2.20	0.40
1:E:117:LEU:HD23	1:E:312:ALA:HB3	2.02	0.40
1:F:326:LEU:O	1:F:332:ALA:HB1	2.22	0.40
1:F:84:ALA:O	1:F:88:LEU:HD13	2.22	0.40
1:A:149:THR:O	1:A:150:GLU:CB	2.70	0.40
1:C:187:ASP:HB3	1:C:251:PHE:CD2	2.56	0.40
1:C:307:ARG:C	1:C:309:PRO:HD3	2.41	0.40
1:E:322:LEU:HA	1:E:325:ILE:HD12	2.04	0.40
1:B:388:PRO:HG2	1:C:67:PRO:HD2	2.04	0.40
1:C:301:ILE:HG13	1:C:304:PHE:H	1.86	0.40
1:C:317:LEU:HD11	1:C:368:GLY:HA2	2.02	0.40
1:D:347:ASP:O	1:D:394:GLU:HB2	2.20	0.40
1:E:158:VAL:HG12	1:E:214:LEU:HD13	2.03	0.40
1:E:257:VAL:HG21	1:E:297:LYS:HB2	2.02	0.40
1:F:187:ASP:OD1	1:F:187:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/363 (86%)	298 (96%)	14 (4%)	0	100	100
1	B	307/363 (85%)	298 (97%)	8 (3%)	1 (0%)	43	75
1	C	297/363 (82%)	290 (98%)	6 (2%)	1 (0%)	43	75
1	D	308/363 (85%)	301 (98%)	6 (2%)	1 (0%)	43	75
1	E	305/363 (84%)	297 (97%)	8 (3%)	0	100	100
1	F	302/363 (83%)	292 (97%)	9 (3%)	1 (0%)	43	75
All	All	1831/2178 (84%)	1776 (97%)	51 (3%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	154	VAL
1	D	154	VAL
1	C	103	ASP
1	B	231	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/299 (82%)	238 (98%)	6 (2%)	50	75
1	B	250/299 (84%)	248 (99%)	2 (1%)	83	90
1	C	248/299 (83%)	245 (99%)	3 (1%)	74	85
1	D	235/299 (79%)	235 (100%)	0	100	100
1	E	235/299 (79%)	233 (99%)	2 (1%)	81	88
1	F	246/299 (82%)	243 (99%)	3 (1%)	74	85
All	All	1458/1794 (81%)	1442 (99%)	16 (1%)	76	86

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	A	157	ASP
1	A	170	ASP
1	A	243	ILE
1	A	391	GLU
1	A	403	ILE
1	B	170	ASP
1	B	211	LEU
1	C	315	ASN
1	C	386	ASP
1	C	398	ILE
1	E	109	GLU
1	E	157	ASP

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Mol	Chain	Res	Type
1	F	68	HIS
1	F	103	ASP
1	F	148	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	101	ASN
1	A	114	ASN
1	B	209	GLN
1	C	101	ASN
1	C	174	GLN
1	C	315	ASN
1	C	406	GLN
1	D	73	HIS
1	D	94	ASN
1	D	114	ASN
1	D	209	GLN
1	E	114	ASN
1	E	209	GLN
1	E	260	HIS
1	F	73	HIS
1	F	81	GLN
1	F	101	ASN
1	F	114	ASN
1	F	160	ASN
1	F	260	HIS
1	F	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	600	-	25,29,29	1.18	3 (12%)	25,45,45	1.82	5 (20%)
3	SO4	A	700	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	A	701	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	A	705	-	4,4,4	0.18	0	6,6,6	0.08	0
2	ADP	B	601	-	25,29,29	1.18	2 (8%)	25,45,45	1.80	5 (20%)
3	SO4	B	702	-	4,4,4	0.18	0	6,6,6	0.06	0
3	SO4	B	707	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	B	708	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	B	709	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	C	500	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	C	703	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	C	704	-	4,4,4	0.17	0	6,6,6	0.08	0
3	SO4	C	706	-	4,4,4	0.17	0	6,6,6	0.09	0
2	ADP	D	602	-	25,29,29	1.18	2 (8%)	25,45,45	1.87	5 (20%)
3	SO4	D	710	-	4,4,4	1.04	0	6,6,6	1.62	1 (16%)
2	ADP	E	603	-	25,29,29	1.18	2 (8%)	25,45,45	1.81	5 (20%)
3	SO4	F	500	-	4,4,4	0.15	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	600	-	-	0/12/32/32	0/3/3/3
3	SO4	A	700	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	A	705	-	-	0/0/0/0	0/0/0/0
2	ADP	B	601	-	-	0/12/32/32	0/3/3/3
3	SO4	B	702	-	-	0/0/0/0	0/0/0/0
3	SO4	B	707	-	-	0/0/0/0	0/0/0/0
3	SO4	B	708	-	-	0/0/0/0	0/0/0/0
3	SO4	B	709	-	-	0/0/0/0	0/0/0/0
3	SO4	C	500	-	-	0/0/0/0	0/0/0/0
3	SO4	C	703	-	-	0/0/0/0	0/0/0/0
3	SO4	C	704	-	-	0/0/0/0	0/0/0/0
3	SO4	C	706	-	-	0/0/0/0	0/0/0/0
2	ADP	D	602	-	-	0/12/32/32	0/3/3/3
3	SO4	D	710	-	-	0/0/0/0	0/0/0/0
2	ADP	E	603	-	-	0/12/32/32	0/3/3/3
3	SO4	F	500	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	ADP	C2-N3	2.01	1.35	1.32
2	E	603	ADP	C2-N3	2.08	1.35	1.32
2	D	602	ADP	C2-N3	2.09	1.35	1.32
2	A	600	ADP	O4'-C1'	2.10	1.44	1.41
2	B	601	ADP	C2-N3	2.14	1.35	1.32
2	A	600	ADP	C5-C4	3.26	1.47	1.40
2	B	601	ADP	C5-C4	3.34	1.48	1.40
2	E	603	ADP	C5-C4	3.37	1.48	1.40
2	D	602	ADP	C5-C4	3.40	1.48	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	ADP	N3-C2-N1	-6.00	123.72	128.86
2	A	600	ADP	N3-C2-N1	-5.83	123.87	128.86
2	B	601	ADP	N3-C2-N1	-5.76	123.94	128.86
2	E	603	ADP	N3-C2-N1	-5.60	124.07	128.86
2	D	602	ADP	PA-O3A-PB	-3.85	119.70	132.63
2	E	603	ADP	PA-O3A-PB	-3.77	119.96	132.63
2	A	600	ADP	PA-O3A-PB	-3.50	120.85	132.63
2	B	601	ADP	C4-C5-N7	-3.32	106.20	109.41
2	B	601	ADP	PA-O3A-PB	-3.26	121.66	132.63
2	E	603	ADP	C4-C5-N7	-3.25	106.27	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	ADP	C4-C5-N7	-3.15	106.37	109.41
2	D	602	ADP	C4-C5-N7	-3.14	106.37	109.41
2	E	603	ADP	C4'-O4'-C1'	2.09	112.00	109.83
2	E	603	ADP	C2'-C3'-C4'	2.13	106.70	102.62
2	D	602	ADP	C2'-C3'-C4'	2.16	106.76	102.62
2	B	601	ADP	C4'-O4'-C1'	2.20	112.12	109.83
2	A	600	ADP	C4'-O4'-C1'	2.21	112.14	109.83
2	D	602	ADP	C4'-O4'-C1'	2.23	112.15	109.83
2	B	601	ADP	C2'-C3'-C4'	2.23	106.91	102.62
2	A	600	ADP	C2'-C3'-C4'	2.44	107.29	102.62
3	D	710	SO4	O4-S-O3	3.72	125.40	108.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	ADP	1	0
2	B	601	ADP	3	0
2	D	602	ADP	4	0
2	E	603	ADP	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/363 (88%)	0.40	29 (9%) 9 8	62, 109, 241, 416	0
1	B	315/363 (86%)	0.34	25 (7%) 12 9	63, 120, 211, 373	0
1	C	307/363 (84%)	0.31	20 (6%) 19 15	67, 123, 226, 412	0
1	D	316/363 (87%)	0.58	36 (11%) 5 4	72, 139, 235, 357	0
1	E	313/363 (86%)	0.56	34 (10%) 5 4	74, 146, 301, 440	0
1	F	314/363 (86%)	0.54	34 (10%) 6 4	65, 140, 272, 354	0
All	All	1885/2178 (86%)	0.46	178 (9%) 8 7	62, 130, 249, 440	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	SER	15.7
1	F	223	PRO	11.9
1	D	150	GLU	11.2
1	F	281	ALA	9.2
1	E	106	ASN	9.1
1	F	220	ALA	8.8
1	E	266	SER	8.2
1	F	106	ASN	7.6
1	D	237	GLN	7.6
1	E	156	GLU	7.4
1	D	149	THR	7.3
1	D	151	ALA	7.1
1	A	149	THR	7.0
1	D	238	VAL	6.9
1	C	154	VAL	6.8
1	F	104	THR	6.6
1	F	105	SER	6.6
1	D	62	SER	6.5
1	E	155	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	176	ALA	5.6
1	D	265	GLY	5.6
1	B	151	ALA	5.5
1	B	171	TYR	5.5
1	E	103	ASP	5.4
1	E	237	GLN	5.4
1	D	104	THR	5.3
1	F	107	GLY	5.3
1	C	199	THR	5.3
1	A	103	ASP	5.3
1	D	103	ASP	5.2
1	A	194	ASP	5.1
1	C	197	SER	5.1
1	A	153	TYR	5.0
1	B	101	ASN	4.9
1	B	392	ASP	4.9
1	A	150	GLU	4.9
1	B	390	MET	4.9
1	A	196	PRO	4.7
1	D	264	THR	4.6
1	E	173	VAL	4.6
1	C	289	GLN	4.5
1	E	220	ALA	4.5
1	F	222	VAL	4.5
1	C	195	ASN	4.5
1	E	105	SER	4.3
1	D	403	ILE	4.2
1	C	153	TYR	4.2
1	E	217	GLY	4.2
1	E	392	ASP	4.1
1	C	103	ASP	4.1
1	C	111	GLY	4.0
1	E	104	THR	3.9
1	D	155	GLY	3.9
1	F	282	SER	3.9
1	D	156	GLU	3.9
1	F	234	GLU	3.8
1	B	228	ARG	3.8
1	C	198	ILE	3.7
1	D	186	ILE	3.7
1	A	238	VAL	3.7
1	A	151	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	260	HIS	3.6
1	D	222	VAL	3.6
1	A	155	GLY	3.6
1	F	152	GLY	3.6
1	A	169	CYS	3.6
1	A	204	GLY	3.5
1	A	173	VAL	3.5
1	E	262	VAL	3.5
1	D	390	MET	3.4
1	E	221	ALA	3.4
1	A	171	TYR	3.4
1	F	219	VAL	3.3
1	B	414	GLY	3.3
1	B	254	LEU	3.3
1	E	219	VAL	3.3
1	A	203	SER	3.3
1	D	223	PRO	3.2
1	D	211	LEU	3.2
1	E	188	LYS	3.1
1	A	195	ASN	3.1
1	F	101	ASN	3.1
1	D	254	LEU	3.1
1	C	155	GLY	3.1
1	D	415	LYS	3.1
1	F	153	TYR	3.1
1	B	173	VAL	3.0
1	E	258	ILE	3.0
1	F	200	ARG	3.0
1	E	330	LYS	3.0
1	F	102	GLY	2.9
1	D	162	ILE	2.9
1	D	220	ALA	2.9
1	E	218	THR	2.9
1	C	104	THR	2.9
1	A	280	LYS	2.8
1	E	109	GLU	2.8
1	D	101	ASN	2.8
1	B	286	LEU	2.8
1	D	239	ASP	2.8
1	C	149	THR	2.8
1	D	221	ALA	2.8
1	F	218	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	156	GLU	2.7
1	B	150	GLU	2.7
1	D	331	ASN	2.7
1	F	149	THR	2.7
1	E	153	TYR	2.7
1	F	235	PHE	2.7
1	B	106	ASN	2.6
1	D	152	GLY	2.6
1	F	108	VAL	2.6
1	B	109	GLU	2.6
1	D	105	SER	2.6
1	E	149	THR	2.6
1	A	106	ASN	2.6
1	B	264	THR	2.6
1	A	107	GLY	2.5
1	A	265	GLY	2.5
1	D	147	THR	2.5
1	D	171	TYR	2.5
1	F	347	ASP	2.5
1	F	112	LYS	2.5
1	D	391	GLU	2.5
1	D	253	GLY	2.4
1	B	413	TYR	2.4
1	C	156	GLU	2.4
1	A	200	ARG	2.4
1	A	237	GLN	2.4
1	C	172	ASP	2.4
1	F	258	ILE	2.4
1	F	204	GLY	2.4
1	E	175	LYS	2.4
1	F	203	SER	2.3
1	D	304	PHE	2.3
1	E	205	GLU	2.3
1	A	174	GLN	2.3
1	D	189	ILE	2.3
1	C	174	GLN	2.3
1	B	205	GLU	2.2
1	E	145	ALA	2.2
1	E	265	GLY	2.2
1	E	113	SER	2.2
1	D	207	VAL	2.2
1	E	365	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	404	ASP	2.2
1	A	105	SER	2.2
1	B	153	TYR	2.2
1	F	257	VAL	2.2
1	A	266	SER	2.2
1	C	294	ASP	2.2
1	E	414	GLY	2.2
1	F	284	GLY	2.2
1	B	403	ILE	2.1
1	F	298	PHE	2.1
1	F	253	GLY	2.1
1	E	179	GLY	2.1
1	B	253	GLY	2.1
1	B	105	SER	2.1
1	B	399	ASP	2.1
1	C	392	ASP	2.1
1	E	159	GLU	2.1
1	F	295	LEU	2.1
1	F	405	GLY	2.1
1	B	159	GLU	2.1
1	D	153	TYR	2.1
1	A	257	VAL	2.1
1	B	396	VAL	2.1
1	B	411	LEU	2.1
1	A	172	ASP	2.0
1	E	206	GLY	2.0
1	C	201	ASP	2.0
1	C	344	GLU	2.0
1	F	81	GLN	2.0
1	E	64	LEU	2.0
1	A	392	ASP	2.0
1	B	152	GLY	2.0
1	F	63	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	702	5/5	0.57	0.35	191,191,191,191	0
3	SO4	C	704	5/5	0.66	0.36	233,233,233,233	0
3	SO4	D	710	5/5	0.69	0.43	190,190,190,190	0
3	SO4	C	706	5/5	0.76	0.23	232,232,232,232	0
3	SO4	B	708	5/5	0.79	0.97	231,231,231,231	0
3	SO4	A	705	5/5	0.83	0.19	173,173,173,173	0
3	SO4	B	707	5/5	0.83	0.26	179,179,179,179	0
3	SO4	A	701	5/5	0.83	0.21	168,168,168,168	0
3	SO4	B	709	5/5	0.85	0.54	178,178,178,178	0
4	MG	D	900	1/1	0.85	0.21	107,107,107,107	0
2	ADP	D	602	27/27	0.88	0.34	132,153,162,170	16
4	MG	B	901	1/1	0.88	0.90	115,115,115,115	0
2	ADP	E	603	27/27	0.89	0.29	135,151,159,166	14
2	ADP	A	600	27/27	0.90	0.26	78,93,113,120	9
3	SO4	C	703	5/5	0.91	0.18	169,169,169,169	0
3	SO4	A	700	5/5	0.91	0.23	147,147,147,147	0
2	ADP	B	601	27/27	0.93	0.26	95,119,137,139	10
3	SO4	F	500	5/5	0.95	0.23	96,96,96,96	0
3	SO4	C	500	5/5	0.95	0.25	100,100,100,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.